

Relativistic configuration-interaction calculation of $K\alpha$ transition energies in beryllium-like argon

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Relativistic configuration-interaction calculations have been performed for the energy levels of the low-lying and core-excited states of beryllium-like argon, Ar^{14+} . These calculations include the one-loop QED effects as obtained by two different methods, the screening-potential approach as well as the model QED operator approach. The calculations are supplemented by a systematic estimation of uncertainties of theoretical predictions.

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I. INTRODUCTION

The subject of the present investigation are the $K\alpha$ transitions in beryllium-like ions. In these transitions, an electron changes the principal quantum number from $n = 2$ to $n = 1$, filling the vacancy in the K -shell core in the initial state. These transitions contribute to the most prominent K -shell emission lines of highly charged ions which have been detected in the spectra of nearly all classes of cosmic X-ray sources. In laboratories, moreover, the K -shell emission lines are often used for the diagnostics of hot plasma, notably in magnetic nuclear fusion and tokamaks, and thus help getting useful information about the equilibrium and non-equilibrium charge-state distributions of ions as well as about the electron and ion temperatures. In view of this importance of the $K\alpha$ line for astrophysics and laboratory diagnostics, accurate theoretical predictions are needed for the reliable identification and interpretation of experimental spectral data [1, 2].

In our previous investigations, we performed relativistic configuration-interaction calculations of the $K\alpha$ transitions in lithium-like ions [3] and in beryllium-like iron [4]. In the current work, we extend our calculations to beryllium-like argon to accommodate ongoing experiments on this ion [5–7].

The paper is organized as follows. In the next section, we give a brief outline of our computation method. Sec. III presents the results of our calculations and compares them with the previous theoretical and experimental data. Relativistic units $\hbar = c = 1$ and charge units $e^2/4\pi = \alpha$ are used throughout this paper.

II. METHOD OF CALCULATION

Within the relativistic quantum mechanics, the energy of the system can be determined by solving the secular equation

$$\det\{\langle\gamma_r P J M|H_{\text{DCB}}|\gamma_s P J M\rangle - E_r \delta_{rs}\} = 0, \quad (1)$$

where “det” denotes the determinant of the matrix. H_{DCB} is the no-pair Dirac-Coulomb-Breit (DCB) Hamiltonian,

$$H_{\text{DCB}} = \sum_i h_D(i) + \sum_{i<j} [V_C(i,j) + V_B(i,j)], \quad (2)$$

where the indices $i, j = 1, \dots, N$ numerate the electrons, h_D is the one-particle Dirac-Coulomb Hamiltonian, and V_C

and V_B are the Coulomb and the Breit parts of the electron-electron interaction. It is assumed that H_{DCB} acts in the space of the wave functions constructed from the positive-energy eigenfunctions of some one-particle Dirac Hamiltonian (the so-called no-pair approximation).

The N -electron wave function $\Psi \equiv \Psi(PJM)$ is assumed to have a definite parity P , total angular momentum J , and angular momentum projection M . In the CI method, the eigenfunctions $\Psi(PJM)$ are represented by a finite sum of the configuration-state functions (CSFs) with the same P , J , and M ,

$$\Psi(PJM) = \sum_r c_r \Phi(\gamma_r P J M), \quad (3)$$

where γ_r denotes the set of additional quantum numbers that determine the CSF. The CSFs are constructed as linear combinations of antisymmetrized products of one-electron orbitals ψ_n . The linear coefficients c_r in Eq. (3) and the energy of the corresponding atomic state are obtained by solving the secular equation (1).

The elements of the Hamiltonian matrix are typically calculated as linear combinations of one- and two-particle radial integrals,

$$\begin{aligned} \langle\gamma_r P J M|H_{\text{DCB}}|\gamma_s P J M\rangle &= \sum_{ab} d_{rs}(ab) I(ab) \\ &+ \alpha \sum_k \sum_{abcd} v_{rs}^{(k)}(abcd) R_k(abcd). \end{aligned} \quad (4)$$

Here, a, b, c , and d numerate the one-electron orbitals, d_{rs} and $v_{rs}^{(k)}$ are the angular coefficients, $I(ab)$ are the one-electron radial integrals, and $R_k(abcd)$ are the two-electron radial integrals. Details of our implementation of the CI method are described in the previous papers [3, 4].

In order to obtain accurate theoretical predictions for energy levels, the relativistic energies obtained from the DCB Hamiltonian should be supplemented by the QED corrections. The best accuracy can be presently obtained within the *ab initio* QED method [8]. Practical calculations within this approach started in late 1990s [9, 10]. Because of large technical difficulties, however, such *ab initio* QED calculations are still restricted mainly to low-lying states of helium-like and lithium-like ions [11, 12]. For calculations of more complex atomic systems, one has to rely on one of the simplified treatments of QED effects.

In the present work, we describe the QED effects by means of two different approximate methods. By comparing the results from these approaches, we estimate the uncertainty of our treatment. The first method is based on summing up the self-energy and vacuum-polarization QED corrections calculated for each one-electron orbital in an effective screening potential. The total QED correction for a given many-electron state is then obtained by adding the QED contributions from all one-electron orbitals, weighted by their fractional occupation numbers as obtained from the eigenvectors of the CI calculation. In this method, the QED correction δE_{QED} is given by

$$\delta E_{\text{QED}} = \sum_a q_a [\langle a | \Sigma_{\text{SE}}(\varepsilon_a) | a \rangle + \langle a | V_{\text{VP}} | a \rangle], \quad (5)$$

where the index a runs over all one-electron orbitals contributing to the many-electron state of interest, q_a is the occupation number of the one-electron orbital, Σ_{SE} is the self-energy operator, ε_a is the Dirac energy of the one-electron state a , and V_{VP} is the vacuum polarization potential. The numerical method for calculating the one-loop self-energy and vacuum-polarization matrix elements in a general screening potential used in the present work was developed in Ref. [13]. This approach for treatment of the Lamb shift in atoms was used in our previous studies [3, 4] and similarly by several other authors, and for beryllium-like ions in particular by Chen and Cheng [14]. In the present work we use in fact two different screening potentials in which the one-loop QED corrections are calculated, the core-Hartree (CH) potential and the localized Dirac-Fock (LDF) potential. The definition of these potentials can be found in our previous works [3, 15].

The second method for evaluation of the QED effects is based on the model QED operator h^{QED} formulated recently by Shabaev et al. [16] and implemented in the QEDMOD Fortran package [17]. To this end, we added the model QED operator to the DCB Hamiltonian by modifying the one-electron integrals $I(a, b)$ of Eq. (4) in our CI code by

$$I(ab) \rightarrow I(ab) + \delta_{\kappa_a, \kappa_b} \langle a | h^{\text{QED}} | b \rangle, \quad (6)$$

and where κ_a denotes the relativistic angular quantum number of the state a . If either a or b is a continuum state (i.e., $\max(\varepsilon_a, \varepsilon_b) > m$), the matrix element of h^{QED} is assumed to be zero. The QED correction to the energy level is then identified by taking the difference of the CI eigenvalues with and without the h^{QED} operator.

Our calculations show that QED corrections obtained by the different methods are in good agreement with each other. In the case of core-excited states, the difference between the results remains well within the 1% range. For the ground and valence-excited states, the deviation is slightly larger, on the level of 1-2%. This is explained by the relatively large effect of the mutual screening of the $1s$ electrons by each other, which is not very well described by approximate methods.

In the present work, we use the QED results obtained with the LDF potential as final values of the QED correction and estimate its uncertainty by the maximal difference between the three QED values.

III. RESULTS AND DISCUSSION

In Table I we present the calculated energy levels of the beryllium-like argon, Ar^{14+} . The total energy is given for the ground $1s^2 2s^2 {}^1S$ state, whereas the *relative* energies (with respect to the ground state) are given for the excited states. Our results are compared with the NIST compilation based on experimental and theoretical data [18, 19], with the relativistic many-body perturbation theory calculation by Safronova *et al.* [20] and with the multiconfigurational Dirac-Fock calculation of Cota *et al.* [21], as well as with the experimental results [22].

All our theoretical predictions are supplied with the uncertainties, which include the error estimates for the Dirac-Coulomb-Breit energy as well as for the QED correction. The former estimate is evaluated by analyzing the configuration-interaction results for successively enlarged basis sets. The QED error was obtained by comparing 3 different QED values from different approaches. The estimated accuracy of our theoretical energies of the core-excited states ranges from 10^{-5} to 10^{-4} in relative units, or from 0.002 to 0.02 Rydbergs.

For the valence-excited states, our results are in good agreement with previous calculations [20], experimental data [22], and with the NIST data base [18]. For the core-excited states, however, there are only 3 entries available in the NIST data base and apparently no experimental results. The only detailed theoretical study of these levels was performed in Ref. [21] by the multiconfigurational Dirac-Fock (MCDF) method. Our results are in general agreement with those of Ref. [21], but the differences are well outside our error bars. The largest deviations of about 0.1 Ry are found for the 5P_J states and for the highest core-excited levels. For the other states, the differences are smaller, typically within 0.05 Ry. It might be mentioned that our result for the ${}^1P_1^o$ state is in excellent agreement with the preliminary result of the Paris experiment [5–7].

In Table II we present our theoretical results for the wavelength of the $K\alpha$ transition lines in beryllium-like argon.

IV. CONCLUSION

In summary, we performed relativistic configuration-interaction calculations of the energy levels of the ground, valence-excited and core-excited states in beryllium-like argon, Ar^{14+} . The relativistic Dirac-Coulomb-Breit energies obtained by the configuration-interaction method were supplemented with the QED energy shifts calculated separately. The QED corrections were obtained by two different approximate methods, the screening-potential approach and the model QED operator method. From the comparison of the results of these two approaches we estimated the uncertainty of the overall QED shift. The uncertainty of the Dirac-Coulomb-Breit energies was evaluated by analysing the convergence of the CI results with respect to the number of partial waves and the size of the one-electron basis. The results obtained for the wavelengths of the $K\alpha$ transitions improve previous theoretical predictions and compare favourably with the preliminary

results of the ongoing experiment.

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TABLE I: Energy levels of beryllium-like argon Ar^{14+} , in Rydbergs, $1 \text{ Ry} = 109\,737.315\,685\,39(55) \text{ cm}^{-1}$. Separately listed are the Dirac-Coulomb energy, the Breit correction, and the QED correction. The total energy is presented for the ground state, whereas for all other states the energies relative to the ground state are given. The theoretical contributions are presented multiplied by the reduced mass prefactor μ/m , $1 - \mu/m = 0.00001373$.

Term	J	Coulomb	Breit	QED	Total	NIST ^a	Other theory	Experiment
$1s^2 2s^2 \ ^1S$	0	-758.9231	0.1629	0.1766	-758.5851 (15)			
$1s^2 2s 2p \ ^3P$	0	2.0807	0.0123	-0.0086	2.0844 (9)	2.0839	2.0836 ^b	2.0837 (16) ^d
	1	2.1520	0.0062	-0.0085	2.1497 (12)	2.1493	2.1491 ^b	2.14931 (9) ^d
	2	2.3136	-0.0024	-0.0081	2.3030 (9)	2.3026	2.3025 ^b	2.3025 (11) ^d
$1s^2 2s 2p \ ^1P$	1	4.1287	0.0018	-0.0083	4.1222 (21)	4.1206	4.1150 ^b	4.12096 (18) ^d
$1s 2s^2 2p \ ^3P^o$	1	226.3281	-0.1327	-0.0747	226.1206 (42)		226.151 ^c	
$1s 2s^2 2p \ ^1P^o$	1	227.4630	-0.1492	-0.0745	227.2394 (25)		227.254 ^c	
$1s 2s 2p^2 \ ^5P$	1	226.8624	-0.1200	-0.0834	226.6589 (21)		226.572 ^c	
	2	226.9599	-0.1220	-0.0832	226.7548 (20)		226.668 ^c	
	3	227.0892	-0.1501	-0.0829	226.8562 (20)		226.787 ^c	
$1s 2s 2p^2 \ ^3P$	0	229.0759	-0.1444	-0.0834	228.8481 (21)		228.811 ^c	
	1	229.0664	-0.1264	-0.0832	228.8570 (28)		228.854 ^c	
	2	229.3167	-0.1452	-0.0828	229.0888 (23)		229.067 ^c	
$1s 2s 2p^2 \ ^3D$	1	229.1822	-0.1355	-0.0831	228.9634 (30)		228.971 ^c	
	2	229.0762	-0.1371	-0.0831	228.8560 (35)	229.188	228.880 ^c	
	3	229.1151	-0.1625	-0.0830	228.8696 (35)	228.980	228.917 ^c	
$1s 2s 2p^2 \ ^3S$	1	230.1192	-0.1319	-0.0831	229.9034 (36)	229.912	229.939 ^c	
$1s 2s 2p^2 \ ^3P$	0	230.3550	-0.1097	-0.0835	230.1618 (102)		230.274 ^c	
	1	230.4777	-0.1128	-0.0831	230.2818 (141)		230.390 ^c	
	2	230.6301	-0.1301	-0.0828	230.4172 (181)		230.515 ^c	
$1s 2s 2p^2 \ ^1D$	2	230.4284	-0.1212	-0.0832	230.2240 (120)	230.398	230.303 ^c	
$1s 2s 2p^2 \ ^1P$	1	231.3742	-0.1577	-0.0830	231.1334 (161)		231.256 ^c	
$1s 2s 2p^2 \ ^1S$	0	231.5411	-0.1120	-0.0829	231.3463 (122)		231.410 ^c	

^a NIST data base [18].

^b Safronova *et al.* [20].

^c Costa *et al.* [21].

^d Edlén [22].

TABLE II: Wavelengths of the $K\alpha$ transition lines in beryllium-like iron Ar^{14+} , in Å.

Transition	Wavelength
$1s^2 2s 2p \ ^3P_1 \rightarrow 1s 2s 2p^2 \ ^3P_0$	3.996 57 (18)
$1s^2 2s 2p \ ^3P_2 \rightarrow 1s 2s 2p^2 \ ^1D_2$	3.998 17 (21)
$1s^2 2s 2p \ ^3P_1 \rightarrow 1s 2s 2p^2 \ ^3S_1$	4.001 11 (10)
$1s^2 2s 2p \ ^3P_2 \rightarrow 1s 2s 2p^2 \ ^3S_1$	4.003 80 (10)
$1s^2 2s^2 \ ^1S_0 \rightarrow 1s 2s^2 2p \ ^1P_1^o$	4.010 16 (4)
$1s^2 2s 2p \ ^1P_1 \rightarrow 1s 2s 2p^2 \ ^1S_0$	4.010 43 (22)
$1s^2 2s 2p \ ^1P_1 \rightarrow 1s 2s 2p^2 \ ^1P_1$	4.014 19 (29)
$1s^2 2s 2p \ ^3P_1 \rightarrow 1s 2s 2p^2 \ ^3D_1$	4.017 69 (6)
$1s^2 2s 2p \ ^3P_2 \rightarrow 1s 2s 2p^2 \ ^3P_2$	4.018 18 (5)
$1s^2 2s 2p \ ^3P_0 \rightarrow 1s 2s 2p^2 \ ^3P_1$	4.018 42 (5)
$1s^2 2s 2p \ ^3P_1 \rightarrow 1s 2s 2p^2 \ ^3D_2$	4.019 59 (7)
$1s^2 2s 2p \ ^3P_2 \rightarrow 1s 2s 2p^2 \ ^3D_1$	4.020 41 (6)
$1s^2 2s 2p \ ^3P_2 \rightarrow 1s 2s 2p^2 \ ^3D_3$	4.022 07 (7)
$1s^2 2s 2p \ ^3P_2 \rightarrow 1s 2s 2p^2 \ ^3P_1$	4.022 29 (5)
$1s^2 2s 2p \ ^3P_2 \rightarrow 1s 2s 2p^2 \ ^3D_2$	4.022 31 (7)
$1s^2 2s 2p \ ^1P_1 \rightarrow 1s 2s 2p^2 \ ^3P_2$	4.026 90 (32)
$1s^2 2s^2 \ ^1S_0 \rightarrow 1s 2s^2 2p \ ^3P_1^o$	4.030 00 (8)
$1s^2 2s 2p \ ^1P_1 \rightarrow 1s 2s 2p^2 \ ^1D_2$	4.030 34 (22)
$1s^2 2s 2p \ ^3P_2 \rightarrow 1s 2s 2p^2 \ ^5P_3$	4.058 13 (4)